

# *Snowmass'21 Community Planning Meeting*

Co-organizers: Cho Ng (SLAC), Jean-Luc Vay (Berkeley Lab)

Joint AF-CompF Session (#64)

October 6, 2020

# Timetable (CT)

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- 3:00PM - Introduction [4 min.]
- 3:04PM - Accelerators & beam physics trends - Sergei Nagaitsev [5 min.]
- 3:09PM - Future computer & programming trends - Axel Huebl [5 min.]
- 3:14PM - Present LOIs by section/subsection [7x3minutes = 21 minutes]
  - 3:14 - AI/ML (4 LOIs): Auralee Edelen
  - 3:17 - Physics for Conventional Accelerators (5 LOIs) - Cho Ng
  - 3:20 - Physics for AAC (3 LOIs) - Nathan Cook
  - 3:23 - Cross-cutting Simulation Tools (6 LOIs) - Jean-Luc Vay
  - 3:26 - Standardization and Practice (3 LOIs) - Axel Huebl
  - 3:29 - Community organization (3 LOIs) - David Bruhwiler
  - 3:32 - Quantum Computing (1 LOI) - He Zhang
- 3:35PM - Open session (comments, missing topics, ...) [15 min.]
- 3:50PM - Planning next steps: [10 min.]
  - Interest group meetings
  - Workshops?
  - White papers: how many? Topics?

## DPF Core Principles and Community Guidelines (CP&CG)

- By participating in this meeting, you agree to adhere to the CP&CG
  - **Respect and support community members**
  - **Commit to constructive dialogue and take initiative**
  - Details of what this means, expectations for behavior, and accountability procedures are provided in the CP&CG document linked at:  
<https://snowmass21.org/cpcg/start>
- Everyone is invited to invoke the CP&CG as needed to encourage constructive and supportive collaboration
- The conveners of this meeting are your recommended first point of contact for reports of CP&CG violations occurring here
  - The conveners have received training in the CP&CG and how to handle reports
  - The CP&CG accountability procedure is designed to encourage early intervention and is flexible enough to appropriately address issues ranging from the discourteous to the egregious
  - Please do not hesitate to contact us!
- Snowmass is most successful when everyone's voice can be heard!

[cho@slac.stanford.edu](mailto:cho@slac.stanford.edu)  
[jlvay@lbl.gov](mailto:jlvay@lbl.gov)

# Purpose of Joint Session

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Community Planning Meeting is **to develop plans and steps** and

- Inspire the community about the field, and encourage them to engage broadly in the Snowmass process
- Inform the community about plans from other regions and from related fields and planned Snowmass activities
- Listen to the community
- Provide space for members across the field to talk to each other and to discuss, promote, and develop new ideas
- Establish cross working-group connections and identify gaps



## **Accelerators & beam physics trends**

S. Nagaitsev (Fermilab/UChicago)

GARD ABP roadmap task force:

Z. Huang (SLAC/Stanford), J. Power (ANL), J.-L. Vay (LBNL),  
L. Spentzouris (IIT), J. Rosenzweig (UCLA), P. Piot (NIU)

October 6, 2020

# GARD Thrusts

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- Supports 5 Research Thrusts:
  - Advanced Accelerator Concepts
  - Accelerator and Beam Physics
    - Expanded to include beam instrumentation and controls
  - Particle Sources and Targets
  - RF Acceleration Technology (NC and SC RF)
    - Includes RF sources, NCRF and SRF R&D
  - Superconducting Magnets and Materials
- Support research efforts at:

The ABP thrust supports research efforts at DOE national labs and university grants

# Science is a proposal-driven enterprise

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- We are to bring to DOE/NSF proposals for research and they respond (with guidance, requirements, and/or funding)
  - Accelerator scientists (like all scientists) should be continuously proposing new ideas and experiments
  - HEP GARD program as a whole is to address “Technology Gaps” for HEP; ABP is supported as a small fraction of GARD.
- Our research proposals should address both “Knowledge gaps” and “Technology gaps” in Accelerator and Beam Physics.

## Definitions and vision statement

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- **Accelerator and beam physics** is the science of the motion, generation, acceleration, manipulation, prediction, observation and use of charged particle beams.
- The Accelerator and Beam Physics (ABP) thrust focuses on fundamental long-term accelerator and beam physics research and development.
- The ABP thrust explores and develops the science of accelerators and beams to make future accelerators better, cheaper, safer, and more reliable. Particle accelerators can be used to better understand our universe and to aid in solving societal challenges.

## GARD ABP mission statement

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- The primary scientific mission of the ABP thrust is to address and resolve the Accelerator and Beam Physics Grand Challenges. Other equally important ABP missions are associated with the overall DOE HEP missions:
  - Advance physics of accelerators and beams to enable future accelerators.
  - Develop conventional and advanced accelerator concepts and tools to disrupt existing costly technology paradigms in coordination with other GARD thrusts.
  - Guide and help to fully exploit science at the GARD beam facilities and operational accelerators.
  - Educate and train future accelerator physicists.

## ABP Grand challenges

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- **Grand challenge #1 (beam intensity):** How do we increase beam intensities by orders of magnitude?
- **Grand challenge #2 (beam quality):** How do we increase beam phase-space density by orders of magnitude, towards quantum degeneracy limit?
- **Grand challenge #3 (beam control):** How do we control the beam distribution down to the level of individual particles?
- **Grand Challenge #4 (beam prediction):** How do we develop predictive “virtual particle accelerators”?

Link to Grand Challenges ([a more detailed description](https://docs.google.com/document/d/11XhutaKropA9kToZhrYmCsoDf6oBunhuQ8mPgYhkJiA/edit?usp=sharing)):

<https://docs.google.com/document/d/11XhutaKropA9kToZhrYmCsoDf6oBunhuQ8mPgYhkJiA/edit?usp=sharing>

## ABP research opportunities

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- We have listed various proposed research areas and opportunities to address the four ABP grand challenges in our LOI
  - [https://www.snowmass21.org/docs/files/summaries/AF/SNOWMASS21-AF1\\_AF7\\_S\\_Nagaitsev-056.pdf](https://www.snowmass21.org/docs/files/summaries/AF/SNOWMASS21-AF1_AF7_S_Nagaitsev-056.pdf)
- ABP research facilities are invaluable!
- Education and training is an important part of ABP
- Effective integration of computational and ML tools across facilities
- We are here to collect your input to our ABP research road for the next 10-15 years.

## ABP community-driven roadmap

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- Working group meetings since ~Sep 2018
- Two community information-gathering workshops:
  - Dec 2019 at LBNL: <https://conferences.lbl.gov/event/279/>
  - Apr – June 2020 (Zoom): <https://indico.fnal.gov/event/22709/>
- Workshops considered:
  - Single-particle dynamics, including nonlinearities, and spin dynamics.
  - High-brightness beam generation, transport, manipulation and cooling.
  - Mitigation and control of collective phenomena: instabilities, space charge, beam-beam, etc
  - Advanced accelerator instrumentation and controls.
  - Modeling and simulation tools; fundamental theory and applied math.
  - Early conceptual integration and optimization, maturity evaluation
  - Connections to other GARD roadmaps; synergies with non-HEP programs



## Grand Challenge #4 (beam prediction): How do we develop predictive “virtual particle accelerators”?

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- Developing “virtual particle accelerators” will provide predictive tools that enable fast computer modeling of particle beams and accelerators at unprecedented levels of accuracy and completeness. These tools will enable or speed up the realization of beams of extreme intensity and quality, as well as enabling control of the beam distribution reaching down to the level of individual particles
- The modeling of beams at extreme intensities and levels of quality, and the design of accelerators that deliver them, also call for integrated predictive tools that can take advantage of the largest supercomputers. Full integration of machine learning tools (and their further development when needed) will be essential to speed up the realization and boost the power of virtual particle accelerators.

## GC #4: Promised dividends

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- Deliver an integrated ecosystem of predictive tools for accurate, complete, and fast modeling of particle accelerators and beams.
- Enable virtual accelerators that can predict the behavior of particle beams in accelerators “as designed” or “as built”.
- Provide the predictive tools that will enable or speed up the realization of the beam intensity, quality, and control grand challenges.
- Develop mathematical and algorithmic tools that benefit from — and contribute to — synergistic developments beyond particle beam and accelerator science.
- Maximize the benefits from — and to — ML/AI tools for beam science and accelerator design.

# Future Computer & Programming Trends

Axel Huebl

*Lawrence Berkeley National Laboratory, U.S.*

## **Snowmass Community Planning Meeting**

*Session 64: Computing Needs of the Accelerator Frontier – Oct 6th, 2020*



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

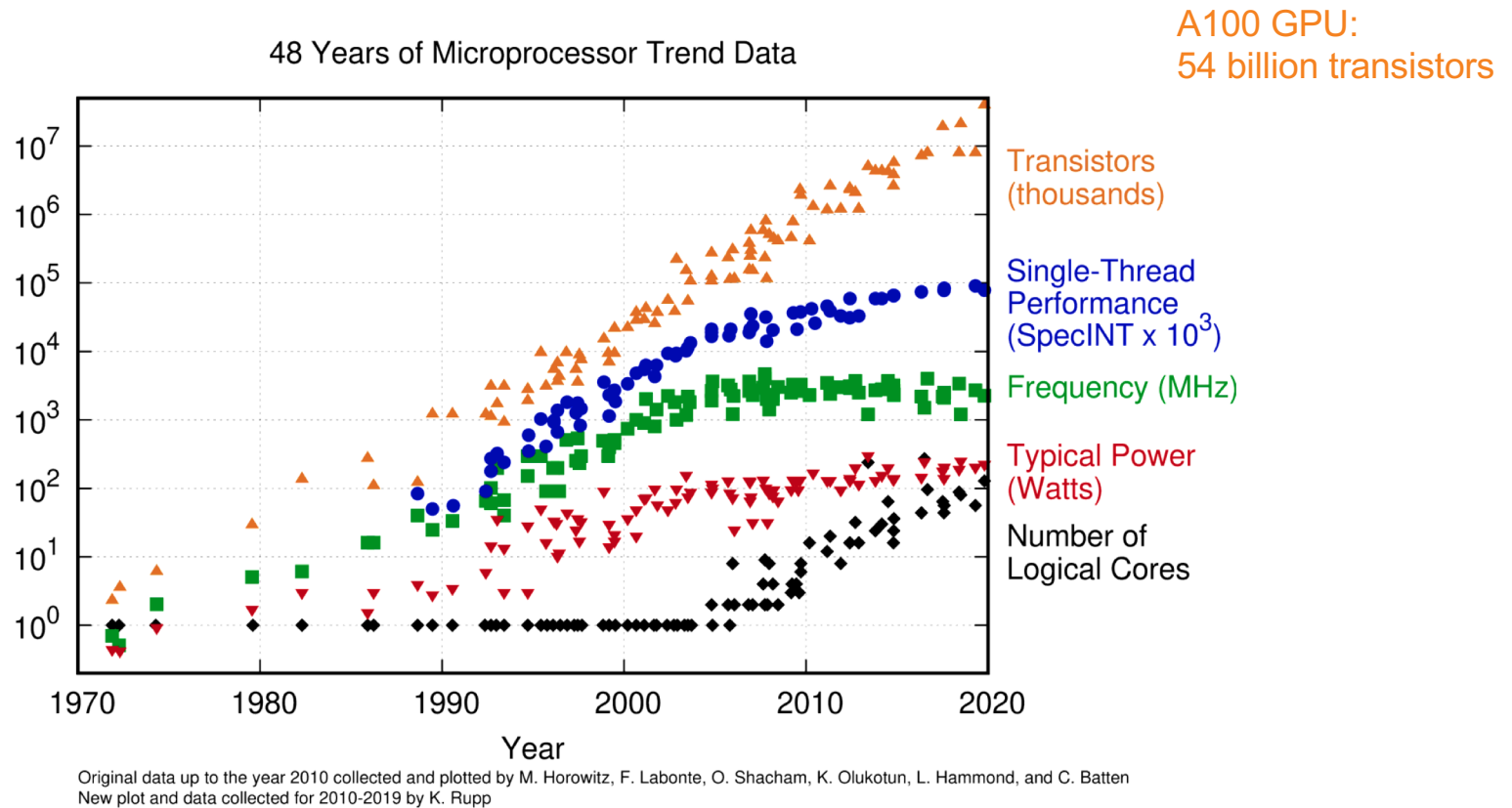


ACCELERATOR TECHNOLOGY &  
APPLIED PHYSICS DIVISION



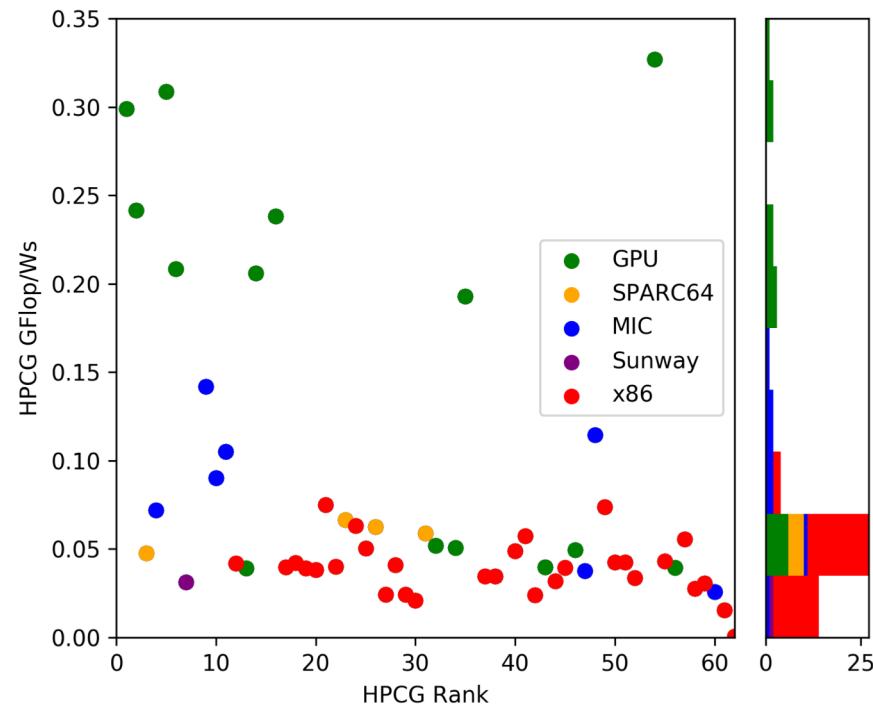
EXASCALE  
COMPUTING  
PROJECT

# 48 Years of Microprocessor Trend Data



<https://www.karlrupp.net/2018/02/42-years-of-microprocessor-trend-data/>

# Power Consumption: HPCG Benchmark



A. Huebl "The Green HPCG List," (11/2018)

[https://plasma.ninja/blog/hpc/manycore/top500/computing/hardware/energy/efficiency/2018/11/18/HPCG\\_Green.html](https://plasma.ninja/blog/hpc/manycore/top500/computing/hardware/energy/efficiency/2018/11/18/HPCG_Green.html)

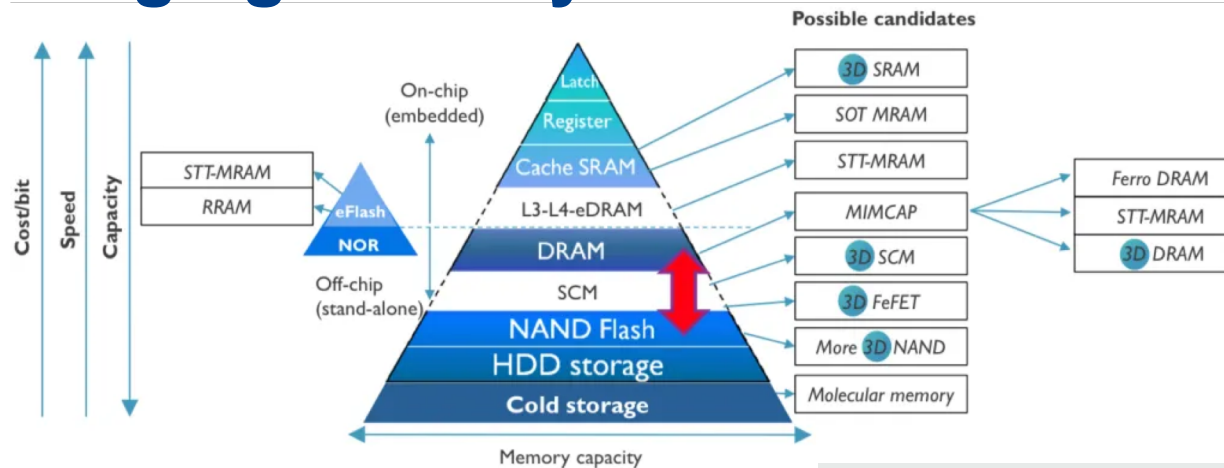
# Growing Divide: Data & Compute



John Backus, 1977 ACM Turing Award:  
„much of that traffic concerns not significant  
data itself, but where to find it“

<https://www.encyclopedia.com/computing/dictionaries-thesauruses-pictures-and-press-releases/non-von-neumann-architecture>; Kapooht, CC-BY-4.0 SA, Wikimedia:Von\_Neumann\_Architecture.svg ; <https://semiengineering.com/a-new-memory-contender/>

# Emerging Memory to Interconnect

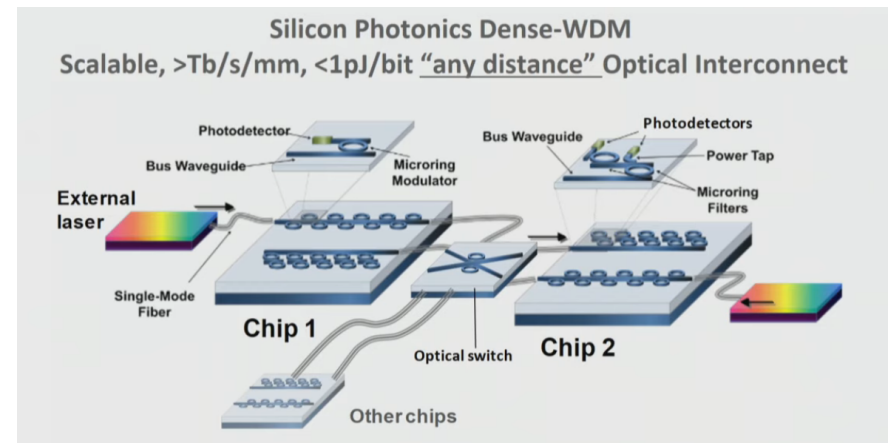


L1 cache reference ..... 0.5 ns  
 Branch mispredict ..... 5 ns  
 L2 cache reference ..... 7 ns  
 Mutex lock/unlock ..... 25 ns  
 Main memory reference ..... 100 ns  
 Compress 1K bytes with Zippy ..... 3,000 ns = 3  $\mu$ s  
 Send 2K bytes over 1 Gbps network ..... 20,000 ns = 20  $\mu$ s  
 SSD random read ..... 150,000 ns = 150  $\mu$ s  
 Read 1 MB sequentially from memory ..... 250,000 ns = 250  $\mu$ s  
 Round trip within same datacenter ..... 500,000 ns = 0.5 ms  
 Read 1 MB sequentially from SSD\* ..... 1,000,000 ns = 1 ms  
 Disk seek ..... 10,000,000 ns = 10 ms  
 Read 1 MB sequentially from disk .... 20,000,000 ns = 20 ms  
 Send packet CA->Netherlands->CA .... 150,000,000 ns = 150 ms

IMEC: <https://semiengineering.com/a-new-memory-contender/>

K. Bergmann "Flexibly Scalable High Performance Architectures with Embedded Photonics" PASC Keynote (2019)

P. Norvig <http://norvig.com/21-days.html#answers> (2012) [https://colin-scott.github.io/personal\\_website/research/interactive\\_latency.html](https://colin-scott.github.io/personal_website/research/interactive_latency.html)



# Today and Near-Term: ~5 years

- **Parallelism:** nodes→devices→rings/SMs→cores→(hyper)threads→SIMD-steps... *on* local→shared→cached→global→remote **memory**

- **Hardware Specialization**

- SIMD: vector to matrix-processing units (tensor cores)
- whole device:

- RISC:

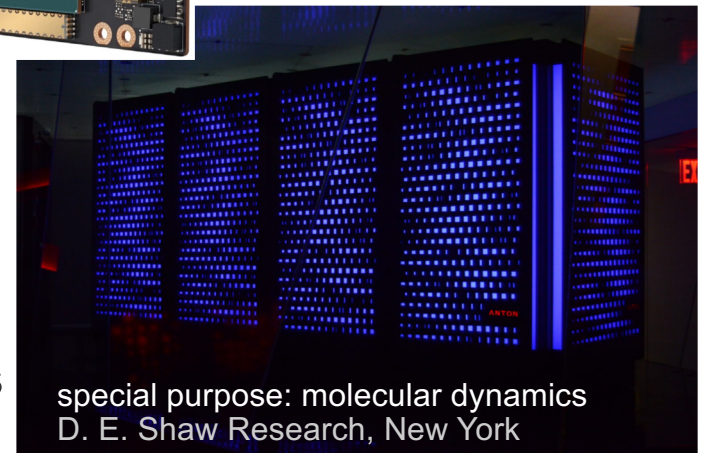
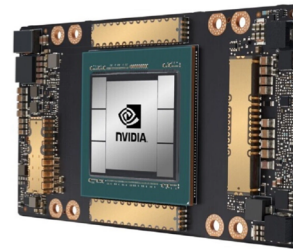
- GPUs: massive parallelism
- ARM / RISC-V / NEC

- FPGAs, DSPs, ...

- ASICs; ANTON2 (2008→2014)

- **Algorithmic Specialization**

- multi-level parallelism; in situ algorithms





## Mid- to Long term: >5-10 years

### ■ Further Specialization

- Programmable FPGAs from *high-level languages* (“HLS”)
- on-**socket** integration of “<5 year” hardware
- *workload-specific* memory & system *designs*

### ■ Programming Models

- *Parallelism* will only rise; potentially to even more levels
- C++23 et al.: Unification of today’s capabilities in standard C++
- Likely emerge of *new paradigms* – for *abstract compute*

### ■ Potentially non-von Neumann *components*

- First signs: FPGAs, DSPs, memory-driven algorithms, neuromorphic chips, ...

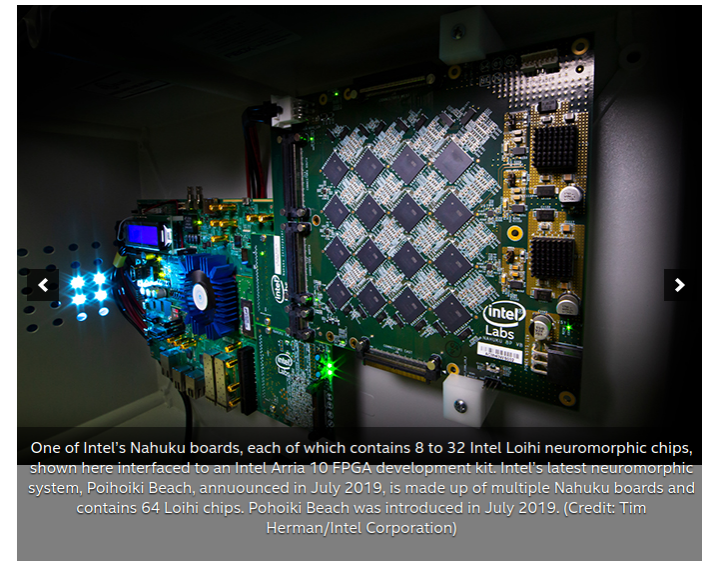
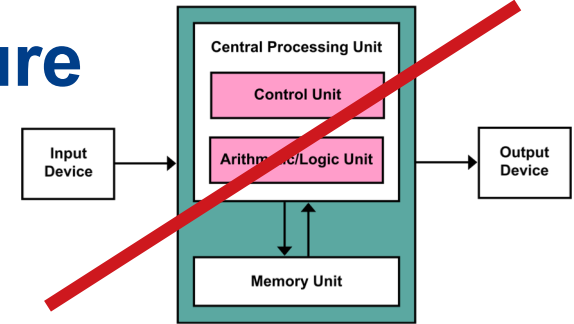
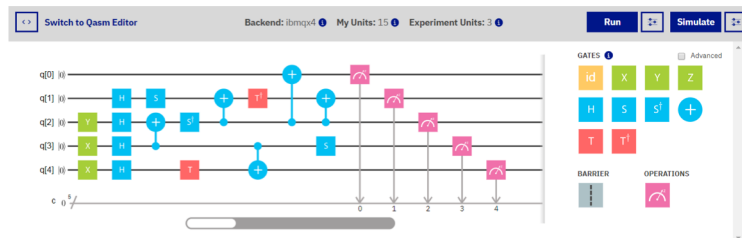
# Beyond von-Neumann Architecture

## Characteristics, e.g.:

- w/o sequential flow of control
- w/o the concept of a named storage variable

## Programming examples (non-procedural):

- declarative (properties)
- data-driven (DSP, analog, quantum gates)



<https://www.encyclopedia.com/computing/dictionaries-thesauruses-pictures-and-press-releases/non-von-neumann-architecture>; Kapooht, CC-BY-4.0 SA, Wikimedia:Von\_Neumann\_Architecture.svg; <https://www.ibm.com/quantum-computing/>; <https://newsroom.intel.com/news/intels-pohoiki-beach-64-chip-neuromorphic-system-delivers-breakthrough-results-research-tests/>

# Potential Routes for Engagement

- **Programming Models:** Need continued community engagement
  - Describe and publish our algorithms and codes
  - Re-design and adopt to industry trends
  - Propose, influence and refine with scientific use-cases
- **Algorithms:** how could a Poisson-solve, PIC-push, advection-diffusion, beam-transport, QED processes be modeled with “X”?
- **Leave comfort zones:** efforts across natural sciences & engineering
- **Adopt:** codes, languages, mental models, unexpected abstractions, ...

# References

- **Future Technologies Group (OLCF)**  
[https://extremecomputingtraining.anl.gov/files/2019/07/ATPESC\\_2019\\_Dinner\\_Talk\\_2\\_7-30\\_Vetter-The\\_Coming\\_Age\\_of\\_Extreme\\_Heterogeneity.pdf](https://extremecomputingtraining.anl.gov/files/2019/07/ATPESC_2019_Dinner_Talk_2_7-30_Vetter-The_Coming_Age_of_Extreme_Heterogeneity.pdf)
- **Supercomputing Conference Panels:** Beyond Von Neumann, Neuromorphic Systems and Architectures
- **PASC 2019 Conference Keynote:** Flexibly Scalable High Performance Architectures with Embedded Photonics (K. Bergman)
- **Intel oneAPI:** FPGA; **SPCL** (ETH Zuerich): FPGA High-Level Synthesis  
**DARPA:** IDEA/POSH Universal Hardware Compiler
- **The Networking & Information Technology Research & Development Program (NITRD),** [nitrd.gov](http://nitrd.gov)
- **TOP500.org** [hpcg-benchmark.org](http://hpcg-benchmark.org)
- **Blogs & online publishing:** [karlrupp.net](http://karlrupp.net) [plasma.ninja/blog](http://plasma.ninja/blog)  
[hpcwire.com](http://hpcwire.com) [thenextplatform.com](http://thenextplatform.com)

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# *Snowmass'21 Community Planning Meeting*

Summary of LOIs on Artificial Intelligence and Machine Learning

*Auralee Edelen (SLAC)*

Joint AF-CompF Session (#64)

October 6, 2020

# List of LOIs

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1. **Machine Learning Meets the Challenges of HEP Research and Development**, Brendan O'Shea, *et al.* [link](#)
2. **Machine learning and Surrogate Models for Simulation-based Optimization of Accelerator Design**, Remi Lehe, *et al.* [link](#)
3. **Application of Machine Learning to Particle Accelerator Simulations**, Daniel Winklehner, *et al.* [link](#)
4. **Adaptive Machine Learning for Time Varying Systems: Noninvasive Diagnostics and Automatic Control for Short Intense Bunches**, Alexander Scheinker, *et al* [link](#)

# Challenges Being Addressed

## Accelerator Optimization / Control

Searching a **high-dimensional, nonlinear parameter space** for highest-quality solutions

- Need to scale to higher dimension, increase search efficiency
  - Unprecedented energy/intensity + stringent beam requirements need new approaches

### Online Tuning/Control

Tune for custom beams  
Compensate for drift/transients

### Design Optimization

Computationally expensive  
Large range of design options

## Beam Measurement / Characterization

**Fine beam control requires excellent beam characterization**  
(*char. also needed for understanding machine*)

- Need non-invasive, high-resolution diagnostics
- Beam exists in 6D phase space, but direct measurements usually limited to a subset; some meas. methods require extra reconstruction steps (e.g. tomography)

## Simulations / Modeling

**Simulations that include nonlinear / collective effects are critical for HEP design and experiment planning**

- These sims are too computationally expensive to use online or in extensive optimization studies
- Sims need to be calibrated to the machine (initial match to measurements + adapt over time)

**Improvement in all of these are critical for meeting future HEP needs (unprecedented beam quality and control\*)**

- Creating, manipulating, and measuring intense and high-power beams
- Control for advanced accelerators (*e.g. higher beam quality in plasma-based accelerators*) and future colliders (*e.g. luminosity, final focus*)

\*e.g. see White and Raubenheimer, doi:[10.18429/JACoW-IPAC2019-THPGW087](https://doi.org/10.18429/JACoW-IPAC2019-THPGW087)



# Proposed Solutions and Benefits to the Community

## Accelerator Optimization

**ML-guided optimization:** iteratively learned information helps select next point (*can leverage previous observations*)

**Combine global models with feedback:** ML model provides initial settings, adaptive feedback + local tuning compensates for prediction errors or drift

**Incorporate expected physics behavior** (*e.g. parameter correlations*) to improve search efficiency

**Safety + uncertainty-aware optimization** (*e.g. avoid beam losses*)

## Simulations / Modeling

**ML surrogate models:** fast-executing stand-ins for expensive simulations

- *Use online and in design, experiment planning, control prototyping*
- *Train on measured data to match machine*

**Adaptive model calibration:** adjust free parameters of models (ML or physics based) with feedback algorithms

## Beam Measurement / Characterization

### Non-invasive “virtual diagnostic” predictions

- ML models or adaptively calibrated physics models (e.g. use or calibrate to other available measurements for prediction)

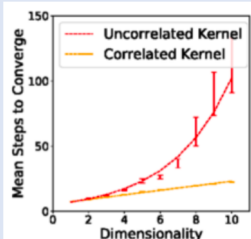
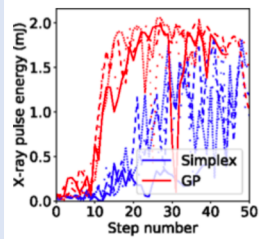
### ML-based reconstruction

- Reconstruct unmeasured parts of phase space
- Improve resolution / quality of standard reconstruction

- **ML critical to discover / exploit patterns that may otherwise go unnoticed + deal with high dimensional data (many variables, images, etc.)**
- **Extraction of practical physics knowledge from operation → feed into future design/control**
- **Expanded benefit from ML algorithm transferability across machines**

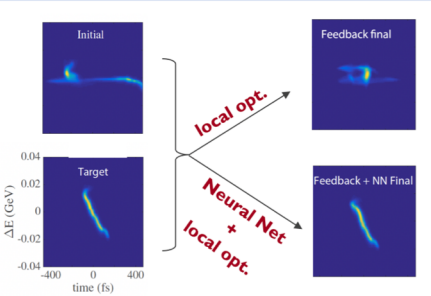
# Proposed Solutions and Benefits to the Community: Examples

## Accelerator Optimization



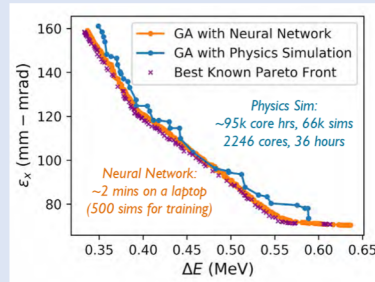
More efficient online optimization with ML + incorporation of physics correlations

*J. Duris, et al, PRL 124, 124801 (2020)*



Warm start from global ML model + local feedback

*A. Scheinker, A. Edelen, et al, PRL, (2018)*

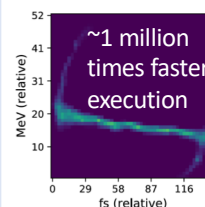


ML-assisted multi-objective optimization (simulation)

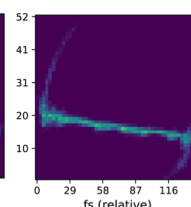
*A. Edelen, et al, PRAB, (2020)*

## Simulations / Modeling

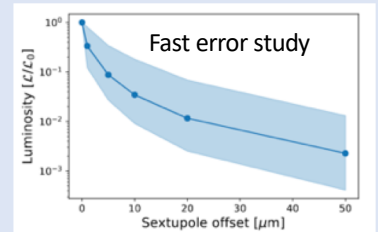
Neural Network



Simulation

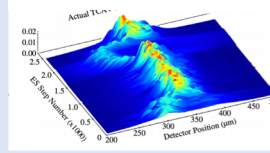


*A. Edelen, et al, NeurIPS 2019*

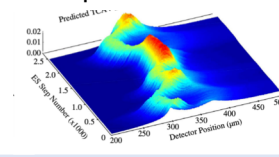


*J. Ogren, et al, arXiv:2009.06454*

Measurement



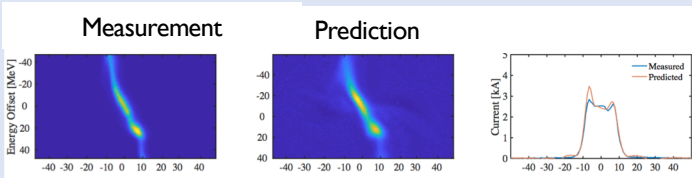
Adaptive Model



Adaptively calibrated physics model

*A. Scheinker, S. Gessner, PRAB 18, 102801 (2015)*

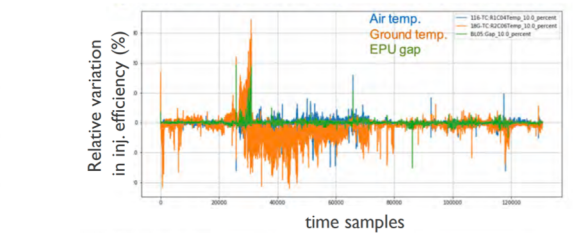
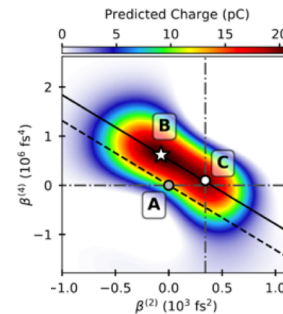
## Beam Measurement / Characterization



Experimental demonstration of non-invasive diagnostic prediction with ML

*C. Emma, A. Edelen, et al., PRAB21, 112802 (2018)*

Discovery aid: extraction of physics info + sensitivities



*Shaloo, et al arXiv:2007.14340*

*F. Wang, X. Huang, NAPAC 2019*

# Synergies, overlaps, and differences between LOIs

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- Combinations of models / approaches improve confidence in predictions and add redundancy
  - Ensemble predictions helps evaluate prediction quality + flag errors
  - Variety of available tuning algorithms useful in different situations (*e.g. requiring more or less previous data: use former in well-explored regions of parameter space, use latter in new regions of parameter space*)
- ML optimization algorithms applicable to both design and online tuning (*with adjustments to suit problem structure, e.g. serial vs. parallel execution*)
- Adaptive feedback methods are broadly useful and can readily couple with global ML models (*e.g. adapting physics or ML models on-the-fly, efficient local tuning to account for drift/modeling errors*)
- ML system models aid optimization / algo prototyping  $\leftrightarrow$  ML guided optimization/sampling can help efficiently build relevant data sets for training

**LOI differences are in specific application and/or approach  $\rightarrow$  all are synergistic and aimed at common goals**

**All need investment in R&D and community infrastructure to realize full potential benefit**

# Synergies, overlaps, and differences with other DOE areas

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- **Shared needs for algorithmic development**

- Many near-identical modeling/optimization challenges across HEP and BES facilities
- Some similar challenges at different facility scales → can prototype at small facilities (e.g. HiRES, Pegasus, AWA) and scale up to larger ones (e.g. FACET-II, LCLS)
- Some specific challenges unique to HEP needs (e.g. tuning for final focus systems for future colliders)

- **Common frameworks** can be applied across DOE facilities for algorithm development and deployment

- Enables broader impact of any one effort
- Much interest in common, community-developed frameworks, but needs funding support

**→ Mutual benefit from joint development efforts, sharing of algorithms, common infrastructure**

# *Snowmass'21 Community Planning Meeting*

## Summary of LOIs on Physics for Conventional Accelerators

R. Gupta, Erdong Wang (BNL), Ao Liu, Ben Freemire (Euclid), E. Barzi, V. Kashikhin, V. Marinozzi (FNAL), D. Davis (Florida State), He Zhang (JLab), Alexander Aleksandrov, Sarah Cousineau, Kiersten Ruisard (ORNL), D. Arbelaez, L. Brouwer, Ji Qiang, T. Shen, R. Teyber, G. Vallone, X. Wang (LBNL), Chengkun Huang, T.J.T. Kwan, Vitaly Pavlenko (LANL), M. Sumption (Ohio State), Zenghai Li, Cho-Kuen Ng (SLAC), B. Cowan (TechX)

Joint AF-CompF Session (#64)

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# List of LOIs

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- **Loss prediction through modeling of high dynamic range beam distributions** - *Kiersten Ruisard, et al.*
- **Electron Cooling Simulation Based on First Principles** - *He Zhang, et al.*
- **Interdisciplinary simulations: Integrating accelerator RF and particle-matter interaction codes** - *Ao Liu, et al.*
- **Physics-based high-fidelity modeling of high brightness beam injectors** - *Chengkun Huang, et al.*
- **Numerical Modeling for Superconducting Accelerator Magnets** - *Lucas Brouwer, et al.*

# Challenges being addressed and scope

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## *High accuracy beam dynamics simulation*

- *Beam halo* simulation from high current beam (10 MW) to determine beam loss effects at 1 part/million level predictive modeling
- Long runtime from slow process of *electron cooling*, accurate electric field calculation and large particle number

## *High fidelity accelerator component modeling*

- Robust geometric interface for integrated modeling of cavity dark current and *radiation* from particle-matter interactions
- *Multi-physics, multi-scale* for start-to-end simulation of microscopic electron transport in material and macroscopic EM in *gun* cavity
- *Multi-physics in magnet* design with static, thermal and mechanical effects in HTS and LTS materials with complex geometric interfaces

# Proposed solution(s) & benefits to community

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- *Measurements and AI/ML algorithms for complete initial beam characterization for accurate beam loss determination in [linacs](#)*
- *Field Poisson solver & fast multipole method for long-range and short-range particle-field dynamics in [electron coolers](#)*
- *Automatic mesh, field and particle transfer in integrated simulation of radiation effects for [machine protection](#) in cryomodules*
- *Integration of electron transport in semiconductor materials and engineered interfaces w/ cavity design for high brightness beam [injectors](#)*
- *FEM modeling including static, thermal, stress and radiation effects for cost effective development of [superconducting magnets](#)*



# Synergies, overlaps & differences

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- Fast and accurate *particle-field interaction algorithms* (e.g. PIC, Poisson) for beam halo and electron cooling modeling of a large particle number
- Verification and validation of new code capabilities from measurements to identify possible missing physics in simulation models
- *Multi-physics, multi-scale* treatment for design and analysis of accelerator components and subsystems – efficient integration of existing codes of different physics
- High fidelity geometric representation of accelerator components and adoption of discretization model crucial for their cost-effective design
- Beam dynamics and component modeling benefiting from *HPC* at emerging architecture with algorithmic development

# *Snowmass'21 Community Planning Meeting*

Summary of LOIs on Advanced Accelerator Concepts Modeling

Nathan Cook (RadiaSoft LLC), Warren Mori (UCLA), Carl Schroeder (LBNL)

Joint AF-CompF Session (#64)

October 6, 2020

# List of LOIs

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- 1. Computational modeling needs of plasma-based accelerators towards future colliders, *Warren B. Mori, Carl B. Schroeder, et al.***
- 2. Modeling of structured plasmas for next generation accelerators, *Nathan M. Cook, et al.***
- 3. Modeling needs for structure wakefield accelerators, *Nathan M. Cook, et al.***

# Challenges being addressed and scope

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- Advanced accelerator technologies will enable future accelerators to meet HEP goals for energy, beam quality, and luminosity.
- These technologies have specialized modeling requirements.
  - *Plasma-based accelerators rely on high fidelity simulations with extreme demands on spatiotemporal resolution to capture beam and plasma response*
  - *Structure-based accelerators leverage intricate material configurations, which impose strict requirements on radiation generation and propagation*
  - *Supporting plasma devices require multi-physics capabilities, ranging from MHD to long-lived kinetic plasma evolution*
- Concerted research efforts are needed to enhance community modeling tools

# Proposed solution(s) & benefits to community

---

- Develop new physics capabilities:
  - Self-consistent high field physics, such as radiation reaction and pair production
  - Hybrid fluid-kinetic modeling to address transitional plasma regimes, including energy deposition
  - High order, self-consistent spectral solvers for long-term, artifact-free simulations and/or symplectic tracking
- Address computational complexity:
  - *Algorithm compatibility for new and heterogeneous architectures and exascale operation*
  - *Mesh refinement and dynamic load balancing to address scale-length disparities*
  - *Improve analysis pipelines for handling increasing (PByte-scale) I/O requirements and cross-compatibility*
- Integrate community efforts
  - *Streamline connections between codes through share I/O and API*
  - *Improved collaborations between labs and university groups to improve development and education pipeline*
- Successful development will permit high fidelity design, optimization, and start-to-end simulation

# Synergies, overlaps & differences

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- Development paths and software practices are synergistic:
  - *All systems benefit from improved workflows, reduced-models, and compatibility with end-to-end virtual accelerator modeling efforts*
- Modeling goals across different physical systems may overlap:
  - *Community code integration, common descriptors and I/O standards , support for novel architectures, improved load balancing techniques*
- Differences arise from physical diversity of systems of interest:
  - *Plasmas require fluid and kinetic physics, structures require dielectric and meta-material fidelity, laser and beam propagation requirements may vary*

# *Snowmass'21 Community Planning Meeting*

## Summary of LOIs on Shared Simulation Tools

Jean-Luc Vay (Berkeley Lab)

Joint AF-CompF Session (#64)

October 6, 2020

# List of LOIs - Shared Simulation Tools

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1. A Parallel Poisson Solver Library for Accelerator Modeling Applications - Ji Qiang, *et al.*
2. Surface Methods for Precision Accelerator Design & Virtual Prototyping of Accelerator Systems - Robert Ryne, *et al.*
3. Beam Dynamics Toolkit - David Sagan, *et al.*
4. A modular community ecosystem for multiphysics particle accelerator modeling and design - Jean-Luc Vay, *et al.*
5. EVA (End-to-end Virtual Accelerators) - Jean-Luc Vay, *et al.*
6. Accelerator and Beam Physics: Grand Challenges and Research Opportunities - Sergei Nagaitsev, *et al.*

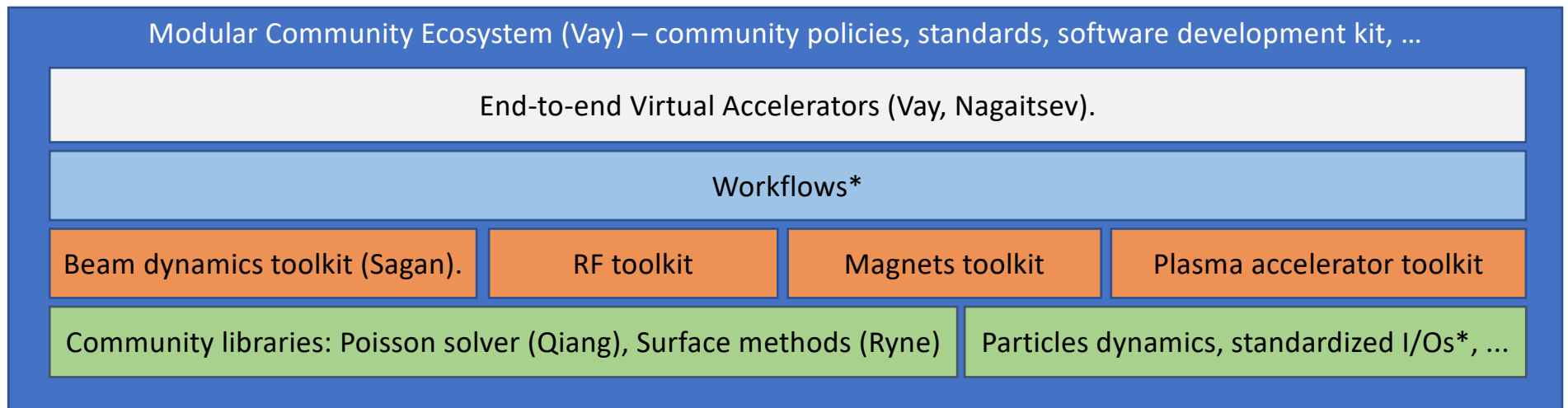


# Challenges being addressed and scope

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- Many simulation tools support the accelerator community but often:
  - lack documentation, hard to modify, duplication (E.g., many beam dynamics codes, Poisson solvers) ;
  - different I/O → hard to compare & combine in multi-physics workflows;
  - coordination is lacking.
- Huge cost to maintain and rewrite as codes die when author moves on.
- Developing efficient tools that run on new hardware (E.g., GPUs) is complex.

# Proposed solution(s) & benefits to community



## Benefits

- Reusable components, portable across platforms (CPUs, GPUs, ...) with single source.
  - ➔ Reduced time for development with better, well benchmarked (less bugs), well documented, well supported and sustainable software stack.
- Easier sharing of data across programs.
- Benefits will extend across entire accelerator community with savings of millions \$.

\*See summary on Cross-Cutting Standardization and Practice – Axel Huebl.

# Synergies, overlaps & differences

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- Coordination of efforts.
- Development of community tools (libraries, toolkits, ecosystem, virtual accelerators).
- Agreement on *permissive open source* licensing\*:
  - Software open source unless need for, E.g., export control.
  - Allows reuse of source & binary code, including for commercial and proprietary applications, fostering collaborations across laboratories, academia and industrial partners.

\*See summary on Cross-Cutting Standardization and Practice – Axel Huebl.

# Standardization and Practice

Axel Huebl

*Lawrence Berkeley National Laboratory, U.S.*

## **Snowmass Community Planning Meeting**

*Session 64: Computing Needs of the Accelerator Frontier – Oct 6th, 2020*



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



ACCELERATOR TECHNOLOGY &  
APPLIED PHYSICS DIVISION

**ATAP**



EXASCALE  
COMPUTING  
PROJECT

# Standardization and Practice (3 LOIs)

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- **Develop/integrate data standards & start-to-end workflows for Accelerator Physics** A. Huebl + 23 (18 inst.)
  - *Predictive capabilities through data & workflow integrations*
- **Aspiration for Open Science in Accelerator & Beam Physics Modeling** A. Huebl + 21 (14 inst.)
  - *Ensuring the scientific method, progress & sustainability*
- **Embracing modern software tools and user-friendly practices, when distributing scientific codes** R. Lehe + 15 (11 inst.)
  - *Improving scientific productivity through code quality & accessibility*

# Data Standards and Start-to-End Workflows

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*Predictive capabilities through data & workflow integrations*

- **Challenges:** long-term ***machines***; diverse codes, ***storage*** & low-level formats; incr. compute-data gap: size & rate; complex ***integrations***
- **Advance: Data**
  - generalize & preserve ***meta-data***; pipelines to ***gateways***
- **Advance: Workflows**
  - flexible ***pipelines*** (code, analysis, incl. in situ); common ***inputs***/DSLs
  - ***workflow languages*** & frameworks: desktop to HPC
- **How:** integrate & contribute to ***standardization***; collaborative ***evolution***

selected success stories

- **openPMD** *an open data model and community*
- **SIMEX, PaNOSC, LUME** *X-FEL facility workflows*

# Aspiration for Open Science

---

- **Definition:** open educational resources, open data, libre/**open source** codes, open methodology, open peer review, documents: open access
- **Reproducibility: *evidence-based research*:** input, code & env.  $\neq$  trivial
- **Open is not Enough:** dedicated people, aspiration for above definitions
- **Continuity/Sustainability:** knowledge transfer, adoptions
- **Collaboration:** within and outside of accelerator & beams
- **Recognized as the most efficient approach for computational science**
  - clear & flexible use/adoption: DOE ASCR; LLNL; most of HEP
  - public money, public science: DOE, EU *and their constituents*

## selected success stories

- **DOE; ASCR; LLNL; LHC/CERN** *ECP SW; PByte Data; ROOT*
- **Commercial/business:** *RedHat Linux, Kitware, NumFocus, Continuum Analytics, QuantStack*

# Modern software tools & user-friendly practices

Embracing tools & best practices when distributing scientific codes

*Our scientific productivity is bound to code quality & accessibility.*

- **Version control and software releases**

- Evolving: track changes; permanent identifiers

- **Documentation:** usage, methods, workflows

- **Accessibility and easy installation**

- `spack/conda/pip install <package>`

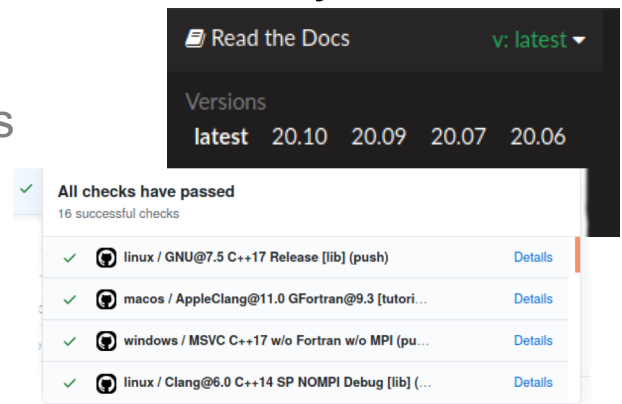
- **User support and communication channels**

- Feedback, improvements, planning: open, accessible, knowledge archive

- **Automated testing:** embrace modifications: simplify verification

selected success stories

- **Sci. Python Ecosystem**     *numpy, matplotlib, tensorflow, ...*
- **HPC Software Stack**     *ECP: xSDK, Spack; various PIC codes*





# *Snowmass'21 Community Planning Meeting*

Summary of LOIs related to Community Organization

David Bruhwiler (RadiaSoft LLC)

Joint AF-CompF Session (#64)

October 6, 2020

# List of LOIs

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- 1. Consortium for PIC Software in Accelerator Science**, *W.B. Mori, T. Antonsen, J. Amundson, J.R. Cary, B. Cowan, D.F. Gordon, K.G. Sonnad, A. Thomas, J. Vieira, et al.*
- 2. Center(s) for Accelerator and Beam Physics Modeling**, *J.-L. Vay, D. Bruhwiler, B. Cros, D. Grote, C.-K. Ng, D. Sagan, M. Thévenet, A. Thomas, H. Vincenti, D. Winklehner, et al.*
- 3. Collaboration between industry and the HEP community**, *D. Bruhwiler, B. Hidding, R. O'Bara, S. Baturin, C.-K. Ng, C.S. Park, P. Piot, A. Sauers, J.-L. Vay, et al.*

# Challenges being addressed and scope

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- Computational challenges facing us are daunting, so we **must** work together.
- How do we work together effectively, without loss of competitive innovation?
- How does the HEP community (labs, universities, industry and DOE) succeed?
  - partial overlap between primary interests & motivations of these community segments
  - partial overlap of interests & motivations between members of each segment
  - partial overlap of interests & activities between DOE/HEP and each institution
  - not primarily a question of DOE/HEP funding decisions, although this is very important
- What changes are required on the part of individual institutions?

# Proposed solution(s) & benefits to community

---

- Create a consortium for PIC software in accelerator science:
  - *Maintain diversity of institutions and scientific/technical approaches*
  - *Facilitate better coordination, including the adoption of technical standards*
  - *Will result in more code benchmarking, physics comparisons, without loss of innovation*
- Create one or more centers for beam physics modeling:
  - *Cultivate (perhaps multi-institutional) centers of expertise in different technical areas*
  - *The rest of the HEP community could then work with and benefit from these centers*
  - *Less duplicated efforts; higher productivity; institutions focus on core competencies*
- More effective integration of industry into community efforts
  - *Enable industry to contribute effectively to software development in multiple areas*
  - *Other community segments can focus on core competencies*
  - *Creates a more diverse set of possibilities with regard to career pipelines*

# Synergies, overlaps & differences

---

- Common theme: find new and better ways to work together as a community
  - *we all agree, and it's an easy thing to say; what are the near-term action items?*
- Common theme: technical standards for file formats, input configuration, physics metadata
- Differences with regard to open source software
  - *there is a recent emphasis on open source software as an ingredient for success*
  - *not everyone agrees and other software licenses continue to thrive*
- Differences with regard to the optimal degree of integration:
  - *relatively loose consortium vs relatively integrated centers of expertise*

# *Snowmass'21 Community Planning Meeting*

## Summary of LOIs on Quantum Computing

He Zhang (Jlab), Ji Qiang, Chad Mitchell (LBNL),  
Ao Liu, Roman Kostin, Ben Freemire (Euclid)

Joint AF-CompF Session (#64)

October 6, 2020

# List of LOIs

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1. **Getting Ready in Algorithm and Software Development for the Arrival of the Quantum Computing Age, *He Zhang, et al.***

# Challenges being addressed and scope

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- *Implement the quantum computing (QC) to enhance our capability for accelerator and beam modeling and simulation.*
- *Quantum computing is developing very fast:*
  - *Hardware: Google announced quantum supremacy.*
  - *Services: Companies provide QC service through cloud.*
  - *Algorithm: many algorithms have been developed. (Linear system solver, ODE/PED solver)*
- *Some building blocks (algorithms, IDEs) are provided, but we still need to build the infrastructure and upper level appliance for accelerator study.*



# Proposed solution(s) & benefits to community

---

- *Proposed solutions:*

- *Develop simulation tools for accelerator physics problems.*
- *Set up QC coding protocols for developers.*
- *Build a community for both users and developers.*

- *Benefits to community:*

- *More powerful and more reliable simulation tools -> better, faster design, deeper understanding in physics.*
- *Promote the development of QC algorithms.*
- *More scientists who master both accelerator physics and QC.*

# Synergies, overlaps & differences

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- *Difference: new emerging computing technique with uncertainties and chances*
- *Common interest:*
  - *Accelerator physics topics: space charge, cooling, etc.*
  - *Machine learning.*
  - *Modern software tools & practices, data standards, workflows, etc.*

# Timetable (CT)

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- 3:00PM - Introduction [4 min.]
- 3:04PM - Accelerators & beam physics trends - Sergei Nagaitsev [5 min.]
- 3:09PM - Future computer & programming trends - Axel Huebl [5 min.]
- 3:14PM - Present LOIs by section/subsection [7x3minutes = 21 minutes]
  - 3:14 - AI/ML (4 LOIs): Auralee Edelen
  - 3:17 - Physics for Conventional Accelerators (5 LOIs) - Cho Ng
  - 3:20 - Physics for AAC (3 LOIs) - Nathan Cook
  - 3:23 - Cross-cutting Simulation Tools (6 LOIs) - Jean-Luc Vay
  - 3:26 - Standardization and Practice (3 LOIs) - Axel Huebl
  - 3:29 - Community organization (3 LOIs) - David Bruhwiler
  - 3:32 - Quantum Computing (1 LOI) - He Zhang
- **3:35PM - Open session (comments, missing topics, ...) [15 min.]**
- 3:50PM - Planning next steps: [10 min.]
  - Interest group meetings
  - Workshops?
  - White papers: how many? Topics?

# Open session (comments, missing topics, ...)

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- Daniel Winklehner.: How to have people to work together?
  - David Sagan: funding!
  - Axel Huebl: people who agree to collaborate.
- Vladimir Shiltsev: Examples of success story?
  - Axel Huebl: openPMD.org
  - Cho Ng: used openPMD for coupling of SLAC ACE3P and LBNL IMPACT
  - JL Vay: work funded in part by CAMPA (Consortium for Advanced Modeling of Particle Accelerators)
  - Rob Ryne: work with David Sagan and Chris Mayes to implement P.S. in BMAD
  - JL Vay: ASCR funded accelerator modeling efforts via SciDAC, Exascale Computing Project
- Auralee: funding for general CSE development of ML software is critical.
- Axel Huebl: we could be more specific on some topics.
- Alex Friedman: based on recent experience of planning meeting for Fusion Energy Sciences, it is important to keep white papers as short as possible.
- Cindy Joe: could we propose something similar to SETI@HOME (implies grid computing / citizen science / public out reach)?

# Chat room

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- 13:52:25 From Axel Huebl (he/him) : Daniel: agreed. Starting with a simple goal, e.g. combining one solver with another - and then automating, documenting and publishing it openly helps a lot to get started.
- 13:56:21 From Daniel Winklehner : True. Another "simple" goal could be to agree on a common format to output/save particle data from simulation codes and then update existing well-established software with this new output option.
- 14:03:23 From Axel Huebl (he/him) : other possible topics for community efforts: integrating ML into our workflows, publishing/exchanging beam data for ML training, etc. Auralee showed many exciting directions.
- 14:07:27 From Cindy Joe : This is rather a tangent, but I have a lot of interest in community integration and outreach. There has been a lot of public interest in efforts like SETI@Home and the protein folding at home, using donated public computer cycles. I wonder if there would be any interest in making computing efforts in our field accessible to do at home in that distributed public way? It would require organization, of course, but could pay off in public support.
- 14:12:42 From Axel Huebl (he/him) : I think that's a fantastic idea, Cindy.
- 14:13:11 From Axel Huebl (he/him) : There are many scientists and citizen scientists that are really interested in using/modifying and experimenting with public codes.
- 14:13:34 From auralee edelen : Agreed re ML workflows Axel. At SLAC for example we use openPMD and an internal h5 data format standard for surrogate model training data sets, which has made it much easier to standardize the ML workflows across different accelerator problems.
- 14:13:56 From auralee edelen : We could do that sort of thing much more broadly across the community for sure.
- 14:14:13 From auralee edelen : Cindy: agreed, that's a great idea!
- 14:14:34 From Frank Tsung : Yes, we have some Jupyter notebooks from the USPAS: <https://github.com/UCLA-Plasma-Simulation-Group/JupyterPIC>
- 14:14:45 From Frank Tsung : Please take a look at those
- 14:15:08 From Axel Huebl (he/him) : Those are great, thanks for sharing those Frank!
- 14:15:40 From Axel Huebl (he/him) : Auralee: maybe some kind of collective "knowledge" portal, e.g. to submit particle beams from various simulations/setups/experiments to - combined with used accelerator/laser regimes as meta-data?
- 14:16:57 From Axel Huebl (he/him) : Too many scenarios are published as figures in papers and really hard to accumulate for meta-studies and comparison with prior results.

# Timetable (CT)

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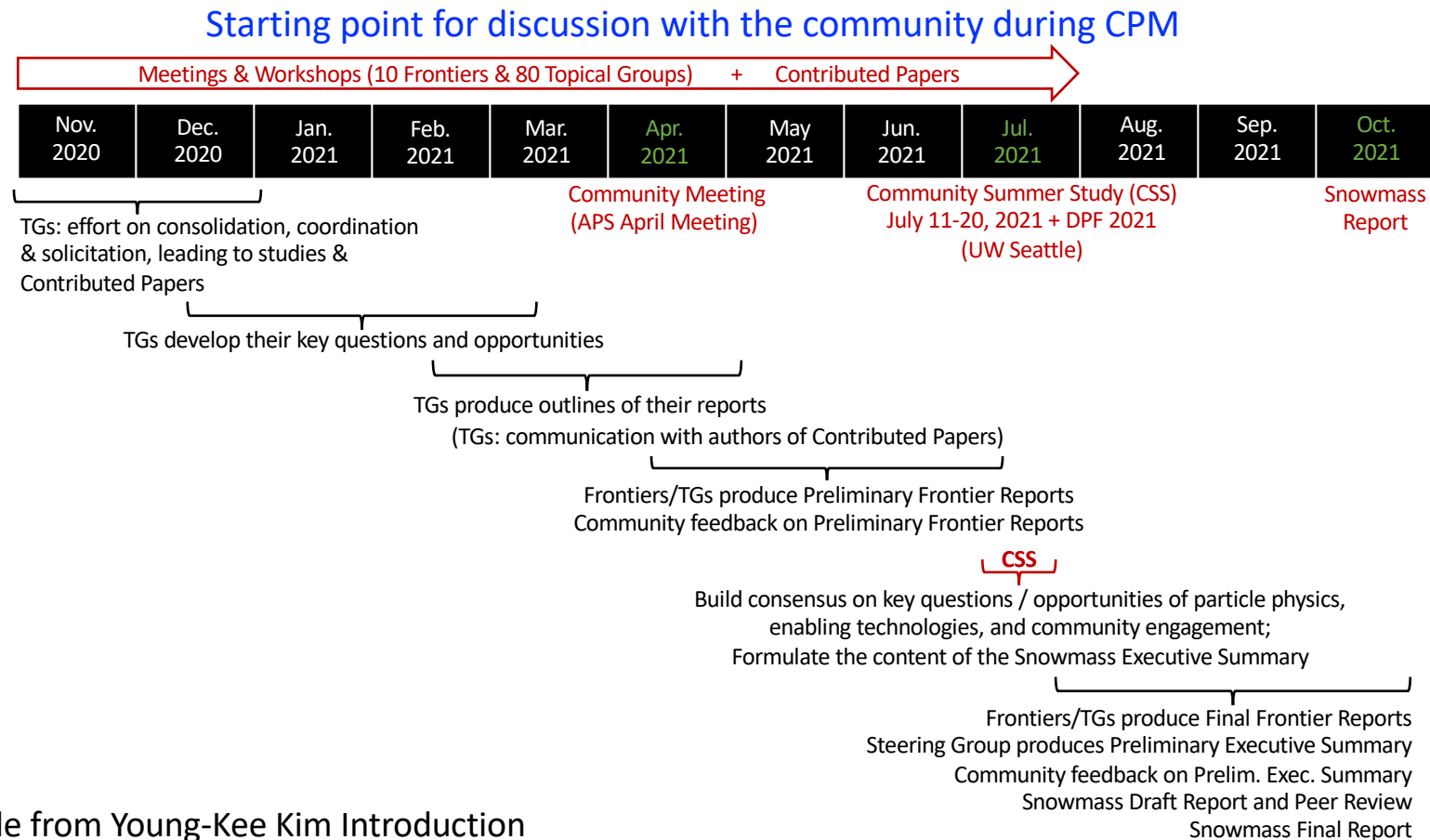
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  - Workshops?
  - White papers: how many? Topics?

# Planning next steps:

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- Beam and Accelerator Modeling Interest Group meetings – Wednesdays @ 1PM-PT
  - Special sessions on
    - Accelerators & beam physics trends
    - Future computer & programming trends
    - AI/ML
    - Physics for Conventional Accelerators
    - Physics for AAC
    - Cross-cutting Simulation Tools
    - Standardization and Practice
    - Community organization
    - Quantum Computing
    - ...
- Workshops?
- White papers: how many? Topics?

# Preliminary Snowmass Timeline / Process



Slide from Young-Kee Kim Introduction



Thanks everyone!!!